

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 715 L/kg

Global applicability domain: Inside

Local applicability domain index: 5.92e-01

Confidence level: 6.79e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Disulfoton sulfone</div> <div>Measured: 1660</div> <div>Predicted: 997</div>	<div>Image not found</div> <div>Disulfoton</div> <div>Measured: 1660</div> <div>Predicted: 1120</div>	<div>Image not found</div> <div>Terbufos sulfoxide</div> <div>Measured: 151</div> <div>Predicted: 239</div>
<div>Image not found</div> <div>Terbufos</div> <div>Measured: 661</div> <div>Predicted: 623</div>	<div>Image not found</div> <div>Phorate</div> <div>Measured: 501</div> <div>Predicted: 588</div>	